Predictive Science Academic Alliance Program (PSAAP)

The slides that follow were presented at the PSAAP Bidder's Meeting May 16-17, 2006 and represent the ASC Trilab authors and interests as presented in the associated White Paper for this subject area.

Materials Stability and Aging

NNSA ASC Predictive Science Academic Alliance Bidders Conference

May 16th, 2006

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Predicting Materials Stability and Aging To Avoid Surprise

The Labs have a mission that requires predictive models of materials aging

- Our systems have a extended lifetime, over 30 years
- Inspection is non-trivial
- Consequence of failure are unacceptable.

There are other industries/missions that have similar constraints – these activities can benefit from fundamental understanding and the resulting predictive capability.

What Other Industries Would Benefit From Materials Aging Models?

- ➢Infrastructure
- ➢Utilities
  - ➢Nuclear power plants
  - ➢Electrical facilities
- ➢NASA
- ➢The Military
  - ➢Ships
  - ➢Planes
- ➢Etc….

Aging Aircraft

Severe cracks found at one nuclear power reactor

How Do We Think About Predicting the Life Cycle of a “System”

Challenges in predicting normal failure rates and the “end of life”:

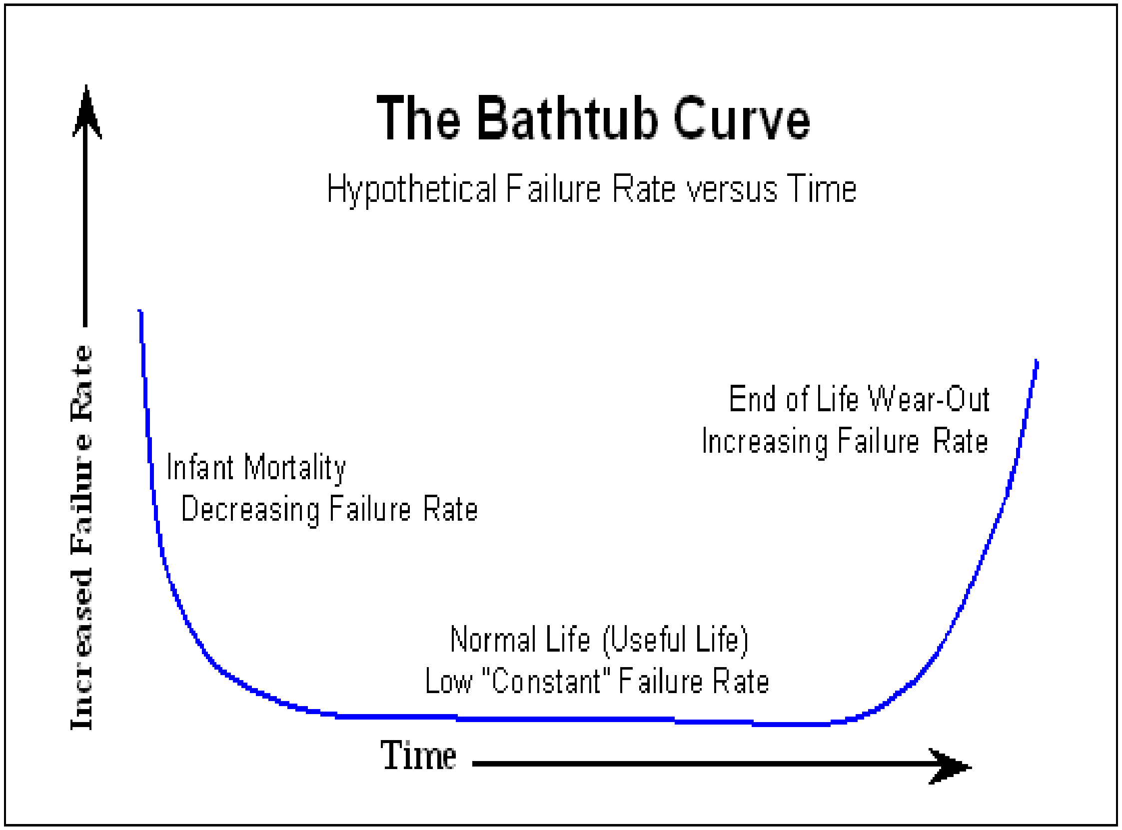
•Accumulation of aging on the overall system is challenge

•Meaningful accelerated aging can be difficult for long “service life” parts and for varying environments.

•Critical physics can change during lifetime.

•Harsh environments present unique challenges.

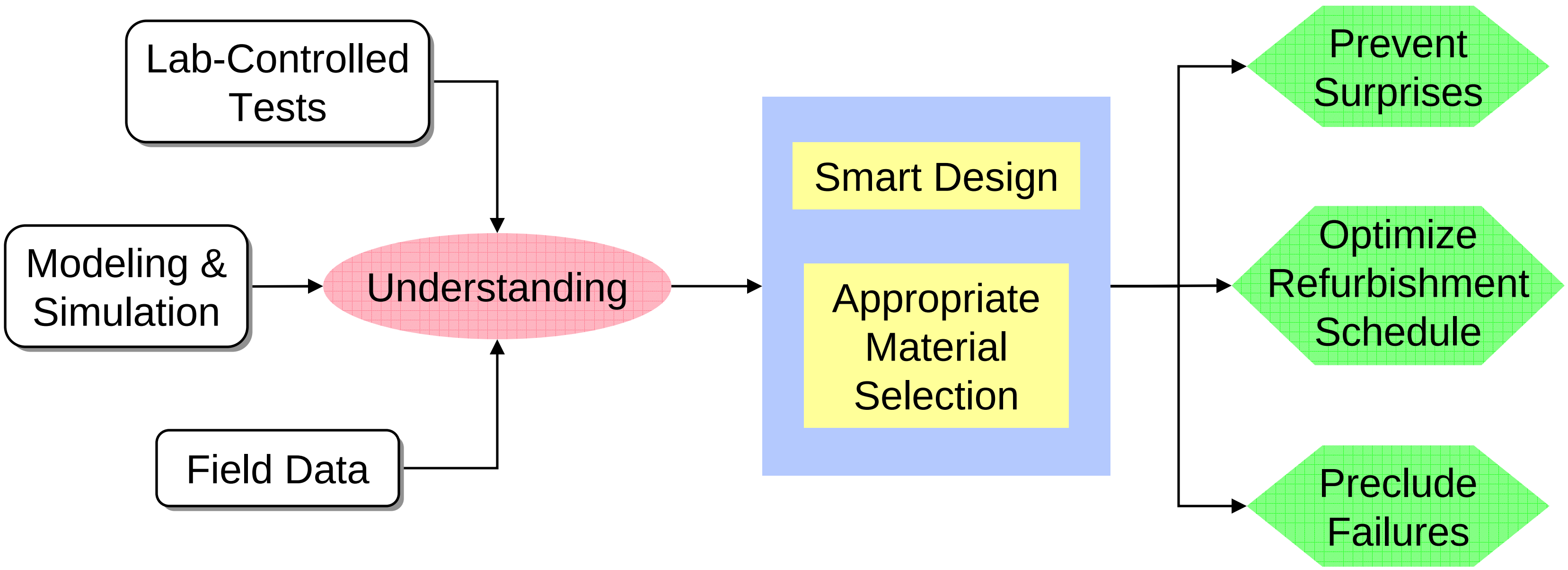
•Embedded components that can’t be easily monitored create challenge.



Aging & Reliability

Material aging is a <u>natural process</u> in a given environment.

- **Change of environment could result in change of aging process.**



What is needed for predictive aging models?

Understand mechanisms of materials aging and failure

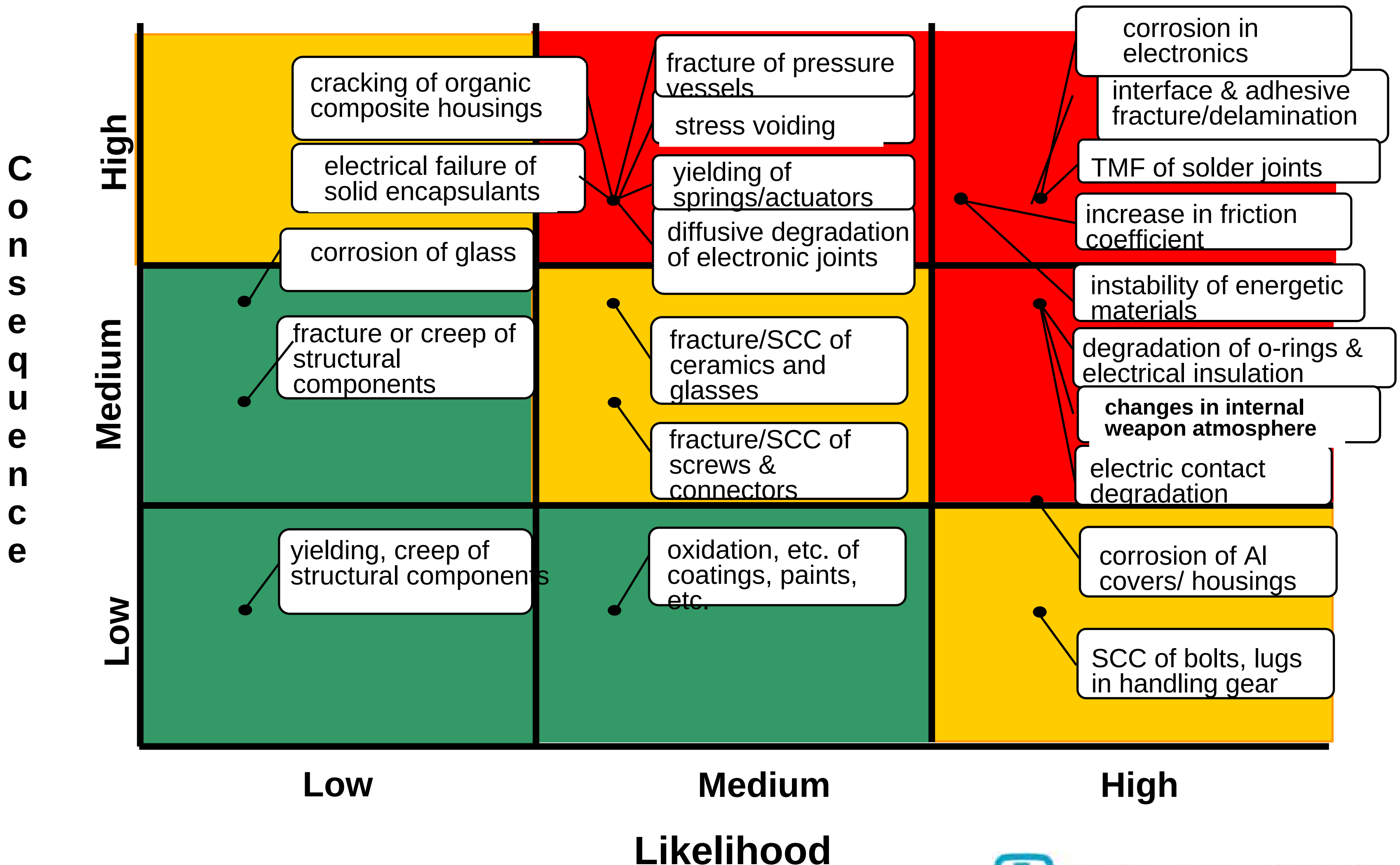
- Establish basic knowledge of how materials age that is useful for addressing reliability and materials performance as a function of age and environment
- Provide physical basis necessary for an effective long-term predictive capability
- Identify how manufacturing processes can introduce latent defects or new materials that may be manifested as an aging concern in the long term

Predict materials changes

- Quantify the effect of material property changes on the desired performance – can result in large computational requirements
- Develop understanding of what and how to monitor effects

Challenges exist in developing the basic phenomena and validating the models.

Setting Priorities for Materials Aging Links the Likelihood and Consequence



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Materials of Interest Are Broad….
A Few Examples

Metals

- Solder
- Corrosion of electrical devices
- Welds
- Lubricants
- Electromechanical contacts
- Thin film metal/metal interfaces

Organics

- O-rings
- Foams and encapsulants
- Silicones
- GMB epoxies
- Adhesive interfaces
- Energetic materials

Inorganics

- Ceramics and glasses
- Dessicants

Fundamental understanding of aging mechanisms and their effects on the materials performance can be challenging:

- Length and time scale challenges
- Multi-physics needs
- Validation challenges

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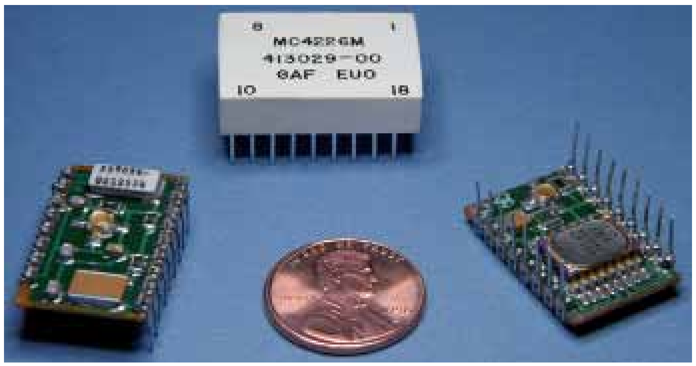
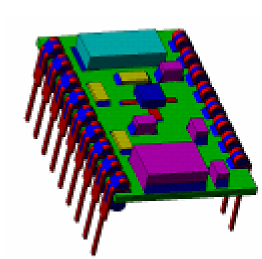
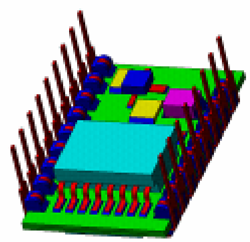
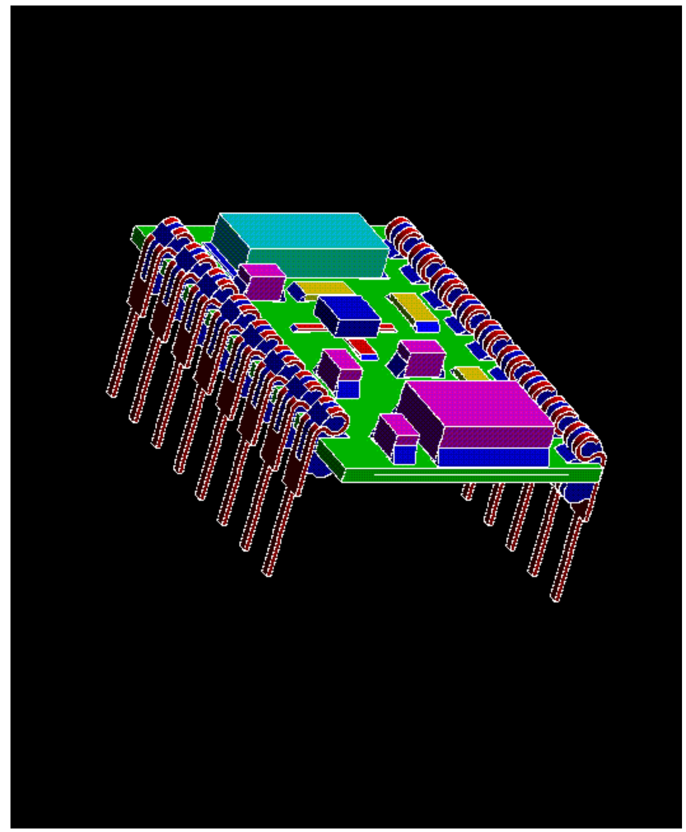
Predicting solder degradation & electronics lifetime is a cross-discipline, multi-scale challenge

One example where we have worked extensively to develop predictive models



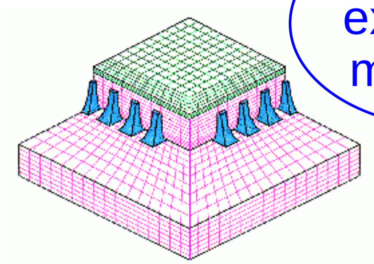






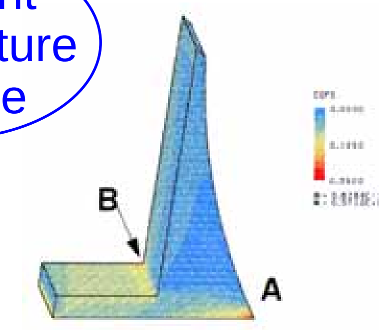
- Circuit board design?
- Loading?
- Material behaviors?
- Operation / storage environment?

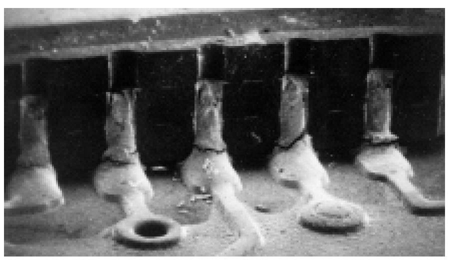
Solder degradation and interconnect failure is a major concern in our business

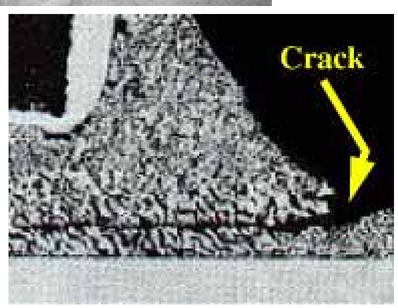


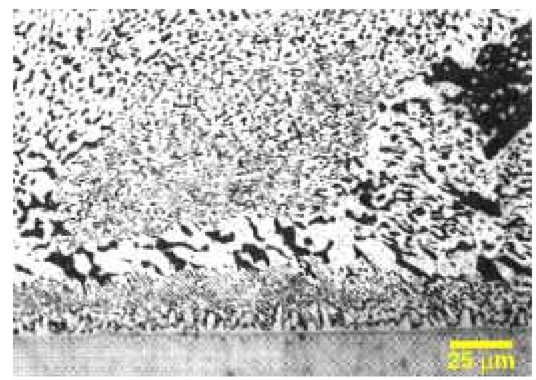
Thermal expansion mismatch → Cyclical strain in the joints ← Ambient temperature change

Cyclical strain in the joints → Heterogeneous microstructural coarsening → Weakening → Final cracking









A multiscale modeling approach was developed to address TMF in solder joints

PI: Liz Holm (SNL/NM)

Integrated, Multiscale Approach:

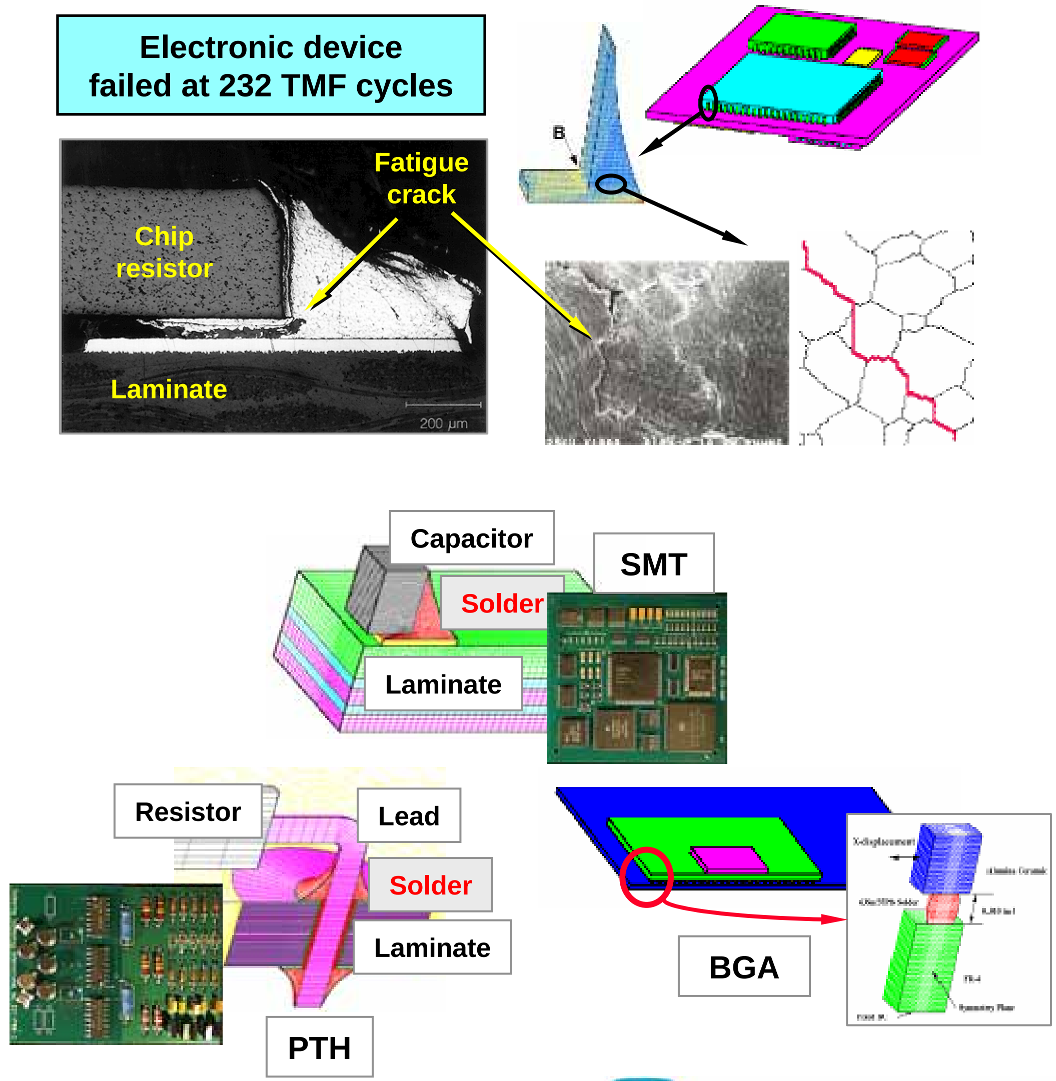
Microscale discovery of failure mechanisms

⬇

Mesoscale FEM/MPM for damage localization

⬇

Macroscale FEM for component lifetime modeling



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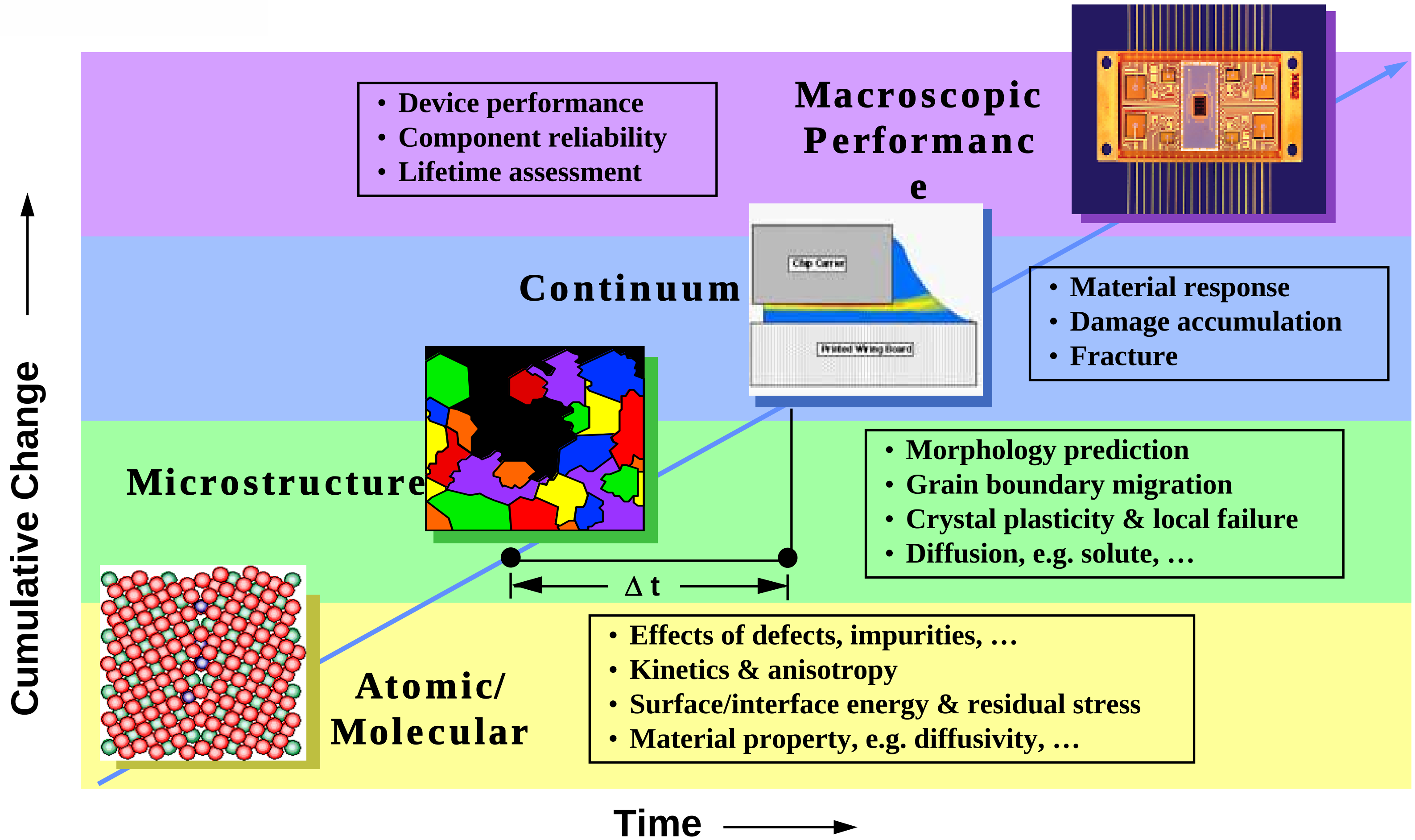
Multiscale materials modeling & simulation
Can play a critical role in predicting materials aging



… there is an increasing need as we seek to understand and control the behavior of increasingly complex materials.

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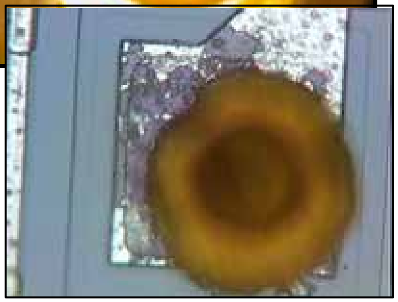
Material Aging Interest Includes Corrosion



Type I – corrosion product layer growth: devices or components that contain copper and/or silver AND

- **a sulfide or ozone-containing gaseous contaminant is present, but**
- **importantly, moisture does NOT have to be present**
- **gas signatures are typically not present due to low concentrations and chemical sinks**

Type II – corrosion voiding: aluminum in microelectronic devices (including hermetic packaged) and nichrome in resistors AND

- **an aggressive contaminant (e.g., halide) and moisture are both present**

Corrosion is difficult to predict because of active/passive nature of engineering alloys, the presence of latent manufacturing defects in product, and the knowledge of the environment (even internal) does not guarantee that we know the local environment in which corrosion occurs.

Predictive Model Challenges:

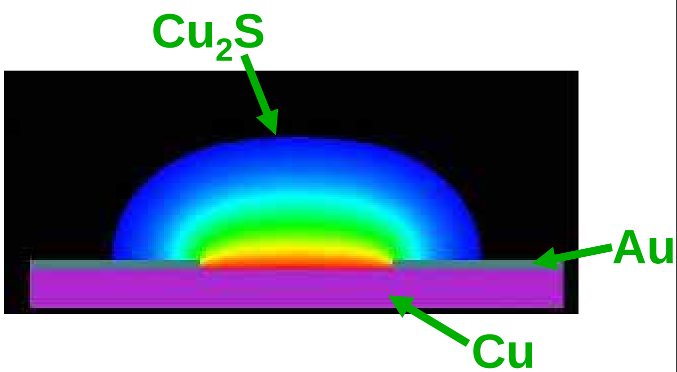
Complex Chemistry, Difficult to validate, Stochastic Nature,

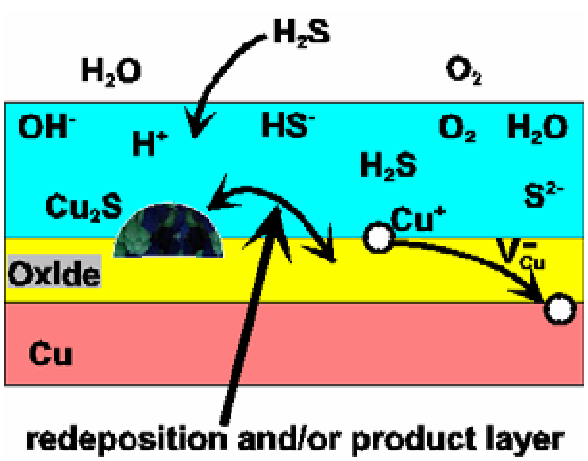
Multiphysics, Bridging Length Scales, etc.

Modeling and Simulation of Corrosion in Microelectronics

Multi-phase reaction/diffusion continuum model is needed to realistically simulate corrosion

Continuum Simulation: Sulfide growth in pinhole





Numerous microscopic processes must be tracked.

Atomistic and quantum mechanical calculations and experimental discovery are used to study the underlying microscopic mechanisms.

- Corrosion product morphology
- Liquid-state chemistry and transport
- Solid-state diffusion

The continuum level models will be used to provide continuum treatment of multi-phase adsorption/chemistry/diffusion.

- Large range of length scales
  - Devices (1000 μm)
  - Sulfide (1 μm)
  - Oxide (0.01 μm)
  - Water layer (0.001 μm)

System level circuit model eventually predicts corrosion effects on system level response.

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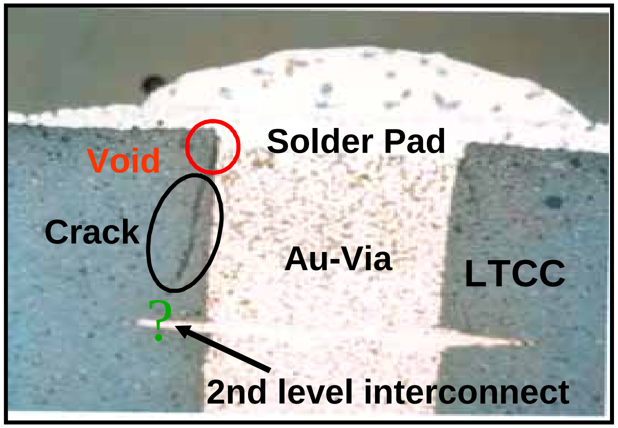
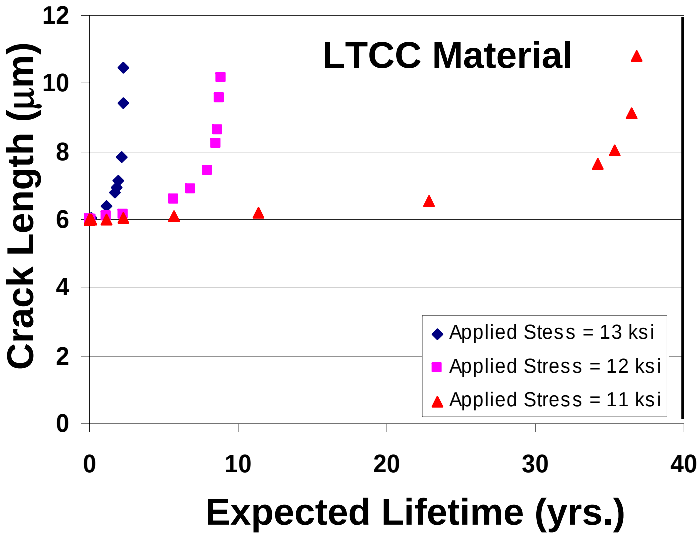
Material Aging Vulnerabilities: Ceramics

- Issue is sub-critical crack growth driven by latent physical defects under mechanical stress, and environmental interactions (e.g., moisture)

- Key preventative aspects include
  - Ensuring stress levels are below material-specific threshold
  - Ensuring stress intensity factor levels are below a material-specific threshold
  - Validating results of modeling using experimental approaches and model samples

Applicable to glass-to-metal seals, battery feed throughs, rack and panel connectors, alumina braze joints, glass ceramics, ferrite ceramics, and PZT





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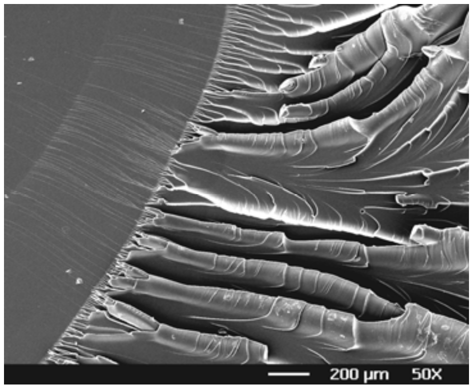
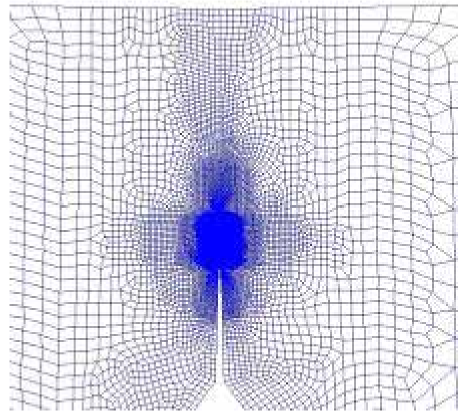
Degradation of Adhesives

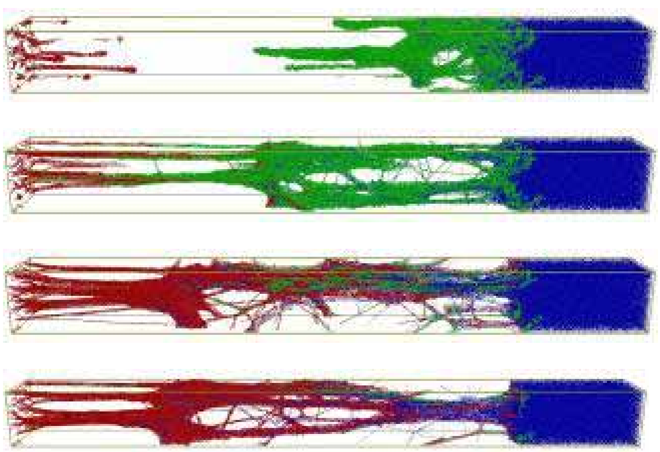
Crack surface in epoxy



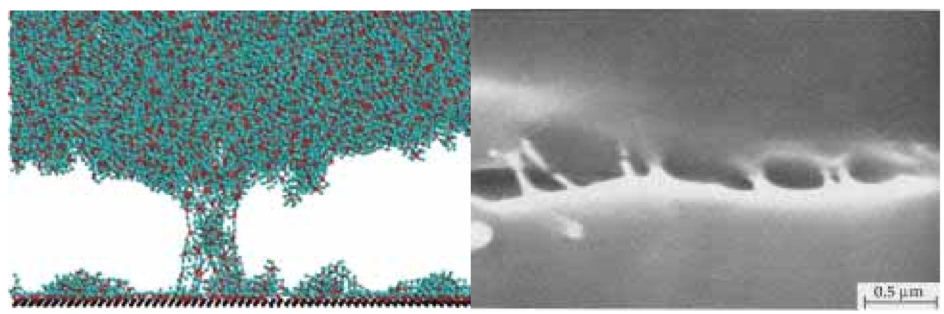
Multscale calculations to predict the degradation & failure of adhesives



Continuum methods to simulate crack initiation and propagation



Simulation of competing failure types in polymer melt



Molecular simulations to examine the nonequilibrium molecular mechanisms

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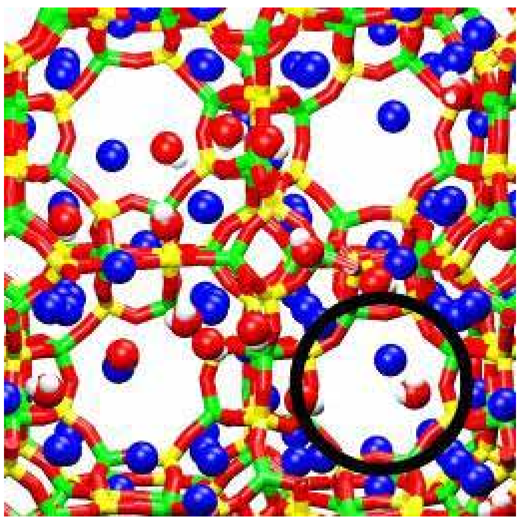
Competitive Adsorption and Reactions in Desiccants

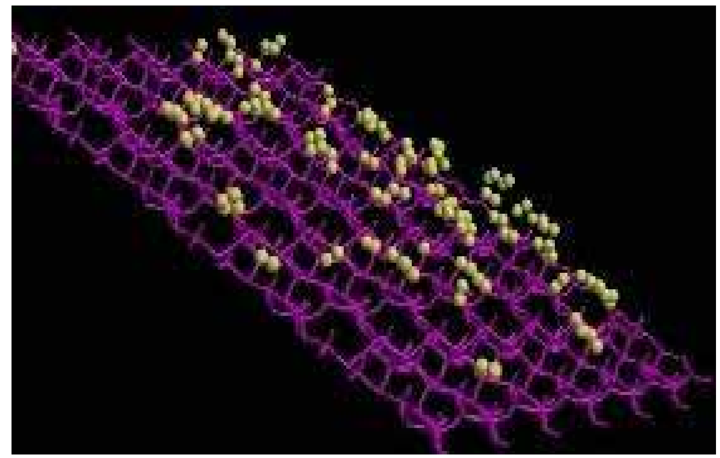
Issues

- Desiccants in weapons systems show unanticipated adsorption behavior.
- Experiments to determine desiccant capacity and lifetime are difficult and costly.



Simulation of chemical reactions in nanoporous desiccant

Adsorption on the surface of desiccant



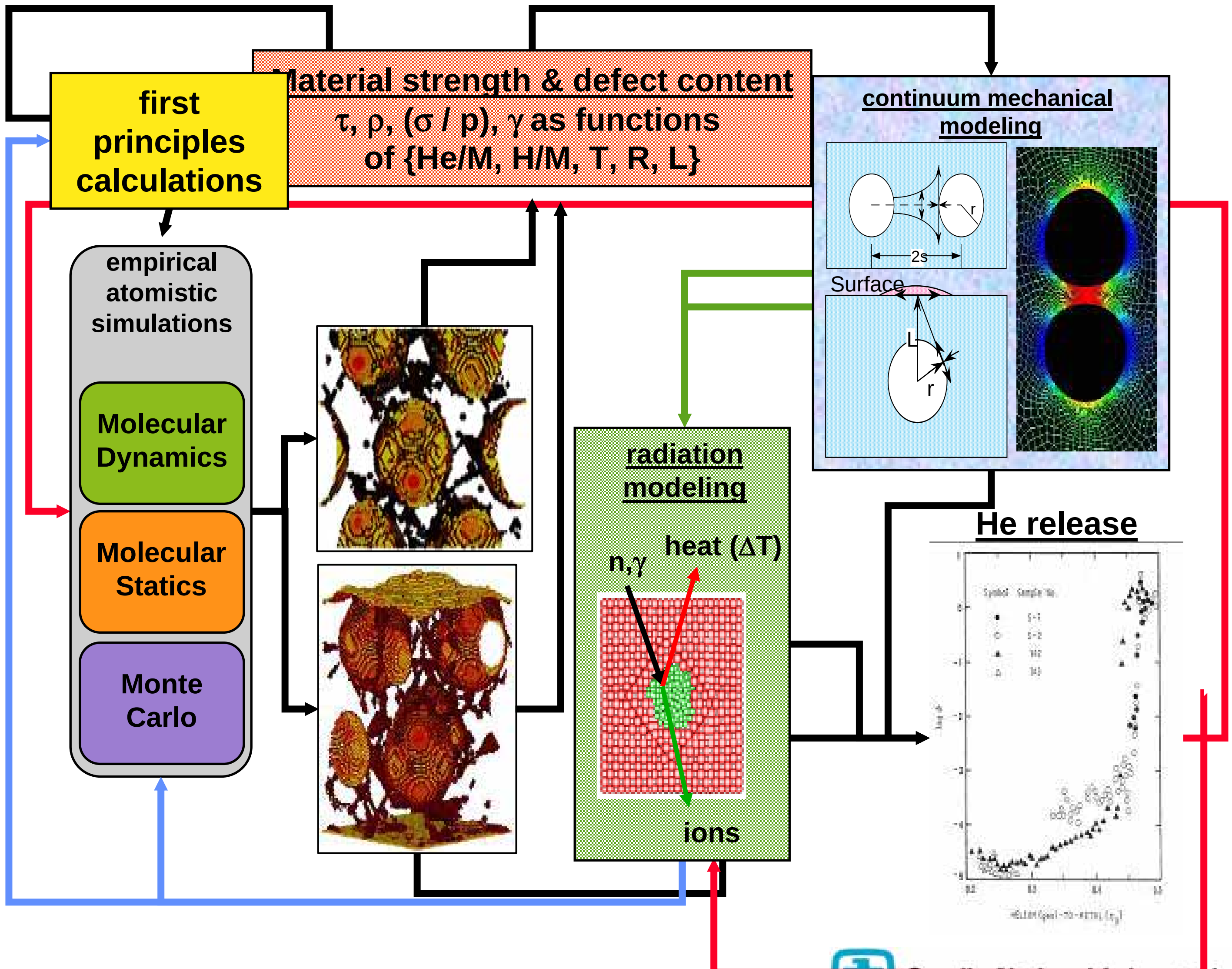
Approach

- Requires multiscale approach to understand fundamental response of materials.
- Use quantum mechanics to investigate chemical interactions inside desiccants and barriers to adsorption due to cations.
- Eventually requires understanding of effects at system level.

Roadmap for Aging and Radiation Effects

Issues

- Helium (He) is a by-product of the decay of tritium. He bubbles grow as the concentration of He increases and eventually cause failure.
- Need to identify criteria for predicting the accelerated release of He from implanted metals and aged hydrides.
- Could eventually be important to the H2 economy



Summary

Developing predictive aging models represents many challenges:

- **Developing fundamental understanding of underlying physics**
- **Validating theories with relevant data**
- **Linking materials processes to materials aging**
- **Novel algorithms and computational tools that allow for long life time simulations**